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Crystal structure of catena-poly[tribenzyl-κ^1C-(μ_2-6-oxidopyridin-1-ium-3-carboxylato-κ^2O:O') tin(IV)-dichloromethane-methanol (1/1/1), C_{29}H_{31}Cl_{2}NO_{4}Sn

Abstract
C_{29}H_{31}Cl_{2}NO_{4}Sn, monoclinic, P2_1/n (no. 14), a = 10.638(4) Å, b = 17.168(7) Å, c = 18.399(5) Å, β = 120.573(16)°, V = 2893.1(18) Å^3, Z = 4, R_{gt}(F) = 0.0314, wR_{ref}(F^2) = 0.0875, T = 298 K.

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The asymmetric unit of the title crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material
A mixture of tribenzyltin oxide (1.6003 g, 2.0 mmol) and 6-hydroxy-nicotinic acid (0.5564 g, 4.0 mmol), in methanol (40 ml) was heated under reflux for 6 h. The obtained clear
solution was evaporated under vacuum. The product was crystallized from a mixture of dichloromethane/ethanol (1:1). Yield 1.8892 g, 73%, m.p. 462 K.

### Experimental details

H atoms were included in the riding model approximation with C–H 0.93–0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C). The O- and N-bound H atoms were refined with O–H = 0.82±0.01 Å and N–H = 0.8686 Å, and with $U_{iso}(H) = 1.5U_{eq}(O)$ or 1.2$U_{eq}$(N).

### Comment

Studies on organotin(IV) compounds having carboxylate ligands with additional donor atom, such as N, O, or S, revealed new structural types which may lead to compounds with different activities [4–8]. In order to exploring whether or not the hetero-atoms (N, O or S) of the carboxylic acid derivatives influence the coordination mode and extension of triaryltin compounds with heteroatom carboxylate ligands this study was undertaken.

In the title compound, the Sn atom exists in a distorted trigonal bipyramidal, surrounded axially by two oxygen atoms and equatorial by the carbon atoms of the benzyl groups. It has an infinite one-dimensional polymeric chain structure, due to the Sn1–O1 and Sn1–O4A [symmetry operation: $x$, $-y$, $z$] distances of 2.153(2) and 2.3391(2) Å, respectively, comparable to a related structure [9]. Translational pseudosymmetry is found in the title structure (klaessengleich, $c/2$). The pseudosymmetry is mainly caused by the solvent molecules. Such a translational
symmetry is an often found feature of reported structures [10].

In detail the distortions from ideal trigonal bipyramidal symmetry for the compound is reflected by the bond angles around the tin atom: C7–Sn1–O1 92.39(10), C7–Sn1–O4A 87.01(10), C14–Sn1–O1 93.04(10), C14–Sn1–O4A 80.10(11), C21–Sn1–O1 96.01(10) and C21–Sn1–O4A 90.48(10), respectively. The bond angle O1–Sn1–O4A is 172.05(8)° which is deviating from the linear angle by 7.95°. The sum of the C7–Sn1–C21 129.26(13), C14–Sn1–C7 115.45(11)° and C14–Sn1–C21 113.93(11)° bond angles is 358.64°, which shows that the atoms of Sn1, C7, C14 and C21 are almost in the same plane. Therefore the tin atom forms a distorted trigonal bipyramidal structure. Due to the protonation at N, a coordination at this site is impossible, which is different to the tribenyltin 4-picoline and similar others [11–14].

There are strong intermolecular N–H⋯O hydrogen bonds (N1–O3 = 2.865 Å) involving pyridinium–N–H and the methanol hydroxyl O atom. There are also intermolecular O–H⋯O hydrogen bonds (O3–O2 = 2.752 Å) [symmetry code: x, −y+0.5, z−0.5] between the methanol hydroxyl O atom and the picolinic carboxyl O atom non-coordinating to Sn center.

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